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A new model for gas radiative properties applicable to oxy-fuel combustion modelling

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Introduction

Radiation is the principal mode of heat transfer in furnaces. Modeling of radiation heat transfer in combustion systems is very complicated. There are two key issues, i.e., how to calculate radiation intensity at different locations along different directions from radiative transfer equations and how to evaluate radiation properties at different locations. Different combustion environments (air-fuel or oxy-fuel) make no difference to the 1st key issue; they will only affect the gaseous radiative properties.

Models for gaseous radiative properties have been well established for air combustion. However, there is uncertainty regarding their applicability to oxy-fuel conditions. In this paper, a new and complete set of models for gaseous radiative properties is derived, which is applicable to CFD modeling of both air-fuel and oxy-fuel conditions. The derivation, calibration and implementation of the new model are given.

Method

- First, a computer code is developed to evaluate the emissivity of *any* gas mixture at *any* condition by using the exponential wide band model (EWBM), and the calculated results are calibrated in very details by data in literature.
- Then, the calibrated code is used to generate emissivity databases for representative air-firing and oxy-firing conditions, for each of which a new weighted-sum-of-gray-gases model (WSGGM) with new parameters is derived. The way to implement the new models into CFD simulations of combustion systems is given.
- Finally, as a demonstration, the new models are applied to CFD modeling of a 0.8MW oxy-natural gas flame furnace. The CFD results are compared with those based on the widely used WSGGMs in literature. Based on that, some useful guidelines on oxy-fuel modeling are recommended.

Result 1: Calibration of EWBM code

Based on “almost exact analytical expressions”, a computer code in c++ is developed to evaluate the emissivity of *any* gas mixture that may consist of H_2O, CO_2, CO, CH_4, NO and SO_2 at *any* condition using the EWBM. The application of this code to a gas mixture is shown below, with almost all the values here calibrated with a reference example.

```
[0] Input Conditions:          Gas temperature,  T_g [K]  =    1500.00
                               Total pressure,   P_T [Pa] = 101325.00
                               Path length,      S   [m]  =    0.50000
                               Mole fraction: (i=0) x_H2O=0.160;  (i=1) x_CO2=0.085;  (i=2) x_CO=0.020;  (i=3) x_CH4=0.005

******************************************** The detailed calculation results ********************************************

[1] Calculate the lower and upper band limits (η_L, η_U) for j-th band of i-th participating species ---------------------
  λ[μm]        χ[g/m2]    Pe      ω[1/cm]   α[m2/(g*cm)]     β        A[1/cm]     τ    Δη=A/(1-τ)[1/cm]  η_L[1/cm]  η_U[1/cm]
 H2O (i=0)
  71.43 (j=0)  11.7090  1.2753  268.398  4327.750522   0.03695  879.403  0.3052  1265.701      0.000    772.850
   6.25 (j=1)  11.7090  1.2753  218.436    41.200000   0.17712  259.220  0.5952   640.322   1279.839   1920.161
   2.66 (j=2)  11.7090  1.2753  232.379    24.995037   0.40010  253.996  0.7334   952.754   3283.623   4236.377
   1.87 (j=3)  11.7090  1.2753  166.926     3.913281   0.17365   45.346  0.9000   453.455   5123.272   5576.728
   1.38 (j=4)  11.7090  1.2753  123.935     2.647639   0.20987   31.001  0.9000   310.011   7094.995   7405.005
 CO2 (i=1)
  14.99 (j=0)  15.1962  1.0178   49.187    19.000000   1.12948  136.241  0.3610   213.219    560.391    773.609
  10.42 (j=1)  15.1962  1.0203   51.898     0.156331   0.90051    2.376  0.9000    23.756    948.122    971.878
   9.43 (j=2)  15.1962  1.0203   39.117     0.158436   2.66500    2.408  0.9000    24.076   1047.962   1072.038
   4.15 (j=3)  15.1962  1.0203   43.377   110.000000   4.45962  201.774  0.2150   257.030   2152.970   2410.000
   2.73 (j=4)  15.1962  1.0165   91.015     5.953672   3.30914   90.473  0.9000   904.730   3207.635   4112.365
   1.92 (j=5)  15.1962  1.0165  133.618     0.138024  12.02135    2.097  0.9000    20.974   5189.513   5210.487
 CO  (i=2)
   4.67 (j=0)   2.2757  1.0016   98.761    20.900000   0.05205   26.148  0.5984    65.118   2110.441   2175.559
   2.35 (j=1)   2.2757  1.0000   77.460     0.181109   0.13722    0.412  0.9000     4.122   4257.939   4262.061
 CH4 (i=3)
   7.63 (j-0)   0.3259  1.0012   81.333    28.000000   2.03872    9.124  0.9000    91.238   1264.381   1355.619
   3.31 (j=1)   0.3259  1.0012  216.887    46.000000   1.53867   14.989  0.9000   149.892   2945.054   3094.946
   2.37 (j=2)   0.3259  1.0012  232.379     4.248850   9.90290    1.384  0.9000    13.845   4213.078   4226.922
   1.71 (j=3)   0.3259  1.0012  174.284     0.811520  23.42482    0.264  0.9000     2.644   5859.678   5862.322

[2] Calculate band transmittances (τ_1, τ_2, τ_b), Planck blackbody fractional function (f_U, f_L), and total emissivity
 η_L[1/cm]   η_U[1/cm]   Overlapped_Bands(i, j)    τ_1      τ_2    τ_b=τ_1*τ_2    f_U       f_L     (1-τ_b)*(f_U-f_L)
    0.000     560.391      ( 0, 0) ( -, -)       0.3052   1.0000   0.3052     1.00000   0.99352      0.004500
  560.391     772.850      ( 0, 0) ( 1, 0)       0.3052   0.3610   0.1102     0.99352   0.98433      0.008176
  772.850     773.609      ( 1, 0) ( -, -)       0.3610   1.0000   0.3610     0.98433   0.98429      0.000027
  773.609     948.122      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.98429   0.97298      0.000000
  948.122     971.878      ( 1, 1) ( -, -)       0.9000   1.0000   0.9000     0.97298   0.97116      0.000181
  971.878    1047.962      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.97116   0.96491      0.000000
 1047.962    1072.038      ( 1, 2) ( -, -)       0.9000   1.0000   0.9000     0.96491   0.96280      0.000212
 1072.038    1264.381      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.96280   0.94346      0.000000
 1264.381    1279.839      ( 3, 0) ( -, -)       0.9000   1.0000   0.9000     0.94346   0.94172      0.000174
 1279.839    1355.619      ( 0, 1) ( 3, 0)       0.5952   0.9000   0.5357     0.94172   0.93282      0.004133
 1355.619    1920.161      ( 0, 1) ( -, -)       0.5952   1.0000   0.5952     0.93282   0.84847      0.034147
 1920.161    2110.441      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.84847   0.81415      0.000000
 2110.441    2152.970      ( 2, 0) ( -, -)       0.5984   1.0000   0.5984     0.81415   0.80616      0.003205
 2152.970    2175.559      ( 1, 3) ( 2, 0)       0.2150   0.5984   0.1287     0.80616   0.80188      0.003730
 2175.559    2410.000      ( 1, 3) ( -, -)       0.2150   1.0000   0.2150     0.80188   0.75599      0.036030
 2410.000    2945.054      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.75599   0.64526      0.000000
 2945.054    3094.946      ( 3, 1) ( -, -)       0.9000   1.0000   0.9000     0.64526   0.61382      0.003144
 3094.946    3207.635      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.61382   0.59031      0.000000
 3207.635    3283.623      ( 1, 4) ( -, -)       0.9000   1.0000   0.9000     0.59031   0.57455      0.001576
 3283.623    4112.365      ( 0, 2) ( 1, 4)       0.7334   0.9000   0.6601     0.57455   0.41325      0.054833
 4112.365    4213.078      ( 0, 2) ( -, -)       0.7334   1.0000   0.7334     0.41325   0.39545      0.004744
 4213.078    4226.922      ( 0, 2) ( 3, 2)       0.7334   0.9000   0.6601     0.39545   0.39304      0.000819
 4226.922    4236.377      ( 0, 2) ( -, -)       0.7334   1.0000   0.7334     0.39304   0.39140      0.000437
 4236.377    4257.939      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.39140   0.38767      0.000000
 4257.939    4262.061      ( 2, 1) ( -, -)       0.9000   1.0000   0.9000     0.38767   0.38696      0.000071
 4262.061    5123.272      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.38696   0.25687      0.000000
 5123.272    5189.513      ( 0, 3) ( -, -)       0.9000   1.0000   0.9000     0.25687   0.24839      0.000848
 5189.513    5210.487      ( 0, 3) ( 1, 5)       0.9000   0.9000   0.8100     0.24839   0.24575      0.000502
 5210.487    5576.728      ( 0, 3) ( -, -)       0.9000   1.0000   0.9000     0.24575   0.20306      0.004269
 5576.728    5859.678      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.20306   0.17432      0.000000
 5859.678    5862.322      ( 3, 3) ( -, -)       0.9000   1.0000   0.9000     0.17432   0.17406      0.000025
 5862.322    7094.995      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.17406   0.08549      0.000000
 7094.995    7405.005      ( 0, 4) ( -, -)       0.9000   1.0000   0.9000     0.08549   0.07076      0.001473
 7405.005   100000.00      ( -, -) ( -, -)       1.0000   1.0000   1.0000     0.07076   0.00000      0.000000
                          -----------------------                                                  ----------------
                          ( -, -) means "no band"                                                  sum = 0.167256724

  The total emissivity of the mixture at the above condition,  ϵ = 0.167256724
  The equivalent (gray) absorption coefficient, -(1/S)*log(1-ϵ)  = 0.366059752
```

The detailed results of the EWBM code applied to calculate the total emissivity of an arbitrary gas mixture.

Result 2: The new models

The complete set of the new models consists of the following equations and new parameters for a number of representative air-fuel and oxy-fuel conditions, and the way to implement them into CFD modeling. Here, only the new WSGGM parameters for the representative oxy-fuel conditions are listed, as seen in Table 1.

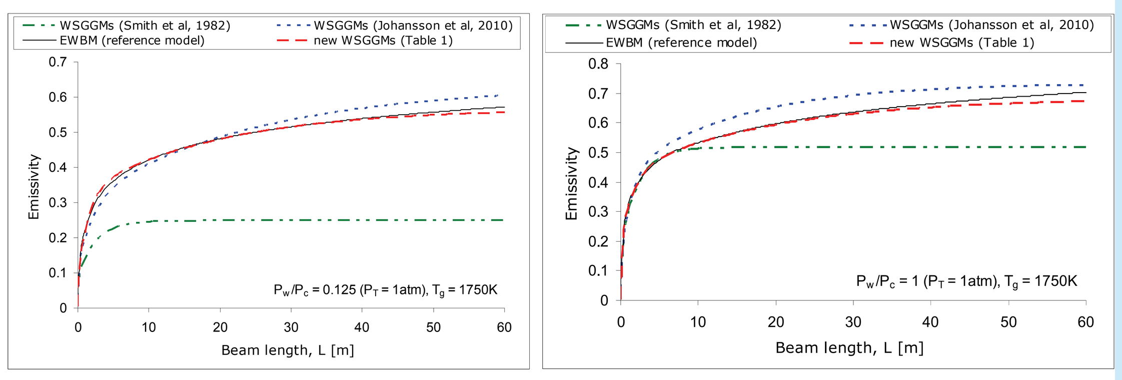
$$\varepsilon = \sum_{i=0}^{I} a_{\varepsilon,i}(T_g)\cdot\left(1-e^{-k_i\cdot P\cdot L}\right)$$

$$\begin{cases} a_{\varepsilon,i}(T) = \sum_{j=1}^{J} b_{\varepsilon,i,j}\left(\dfrac{T_g}{T_{\mathrm{ref}}}\right)^{j-1} \qquad i = 1,\cdots,I \qquad a_{\varepsilon,i} > 0 \\ I = 4,\quad J = 4,\quad T_{\mathrm{ref}} = 1200 \text{ (in the unit of K) for a better estimate} \\ k_0 = 0 : \text{represent 'windows' in the spectrum;}\quad a_{\varepsilon,0} = 1 - \sum_{i=1}^{I} a_{\varepsilon,i} > 0 \\ P: \text{ the sum of the partial pressures of all the participating gases, atm} \end{cases}$$

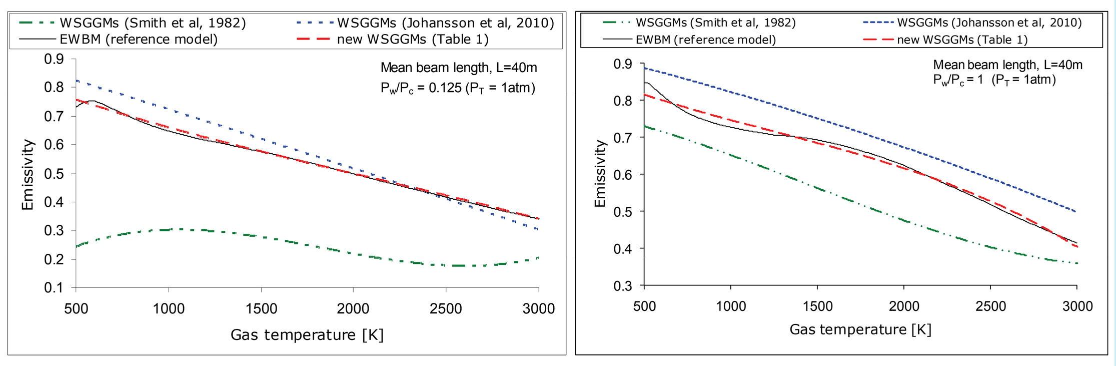
Table 1. New parameters for the WSGGMs, applicable to oxy-fuel flames.

i	k_i	$b_{\varepsilon,i,1}$	$b_{\varepsilon,i,2}$	$b_{\varepsilon,i,3}$	$b_{\varepsilon,i,4}$
$P_w \to 0$ atm, $P_c \to 0$ atm					
1	0.009422	0.778969	-1.342848	0.964858	-0.195747
2	0.415646	-0.011449	0.343754	-0.234886	0.044008
3	11.617018	-0.007627	0.242233	-0.173738	0.033868
4	319.911168	0.080082	-0.049280	0.001861	0.002232
$P_w = 0.1$ atm, $P_c = 0.1$ atm					
1	0.256738	0.492304	-0.433789	0.279329	-0.057770
2	3.108033	0.082686	0.486294	-0.369752	0.070509
3	52.585782	0.144385	-0.083662	0.002003	0.003902
4	440.845718	0.079515	-0.110361	0.051379	-0.007983
$P_w = 0.3$ atm, $P_c = 0.1$ atm					
1	0.132242	0.478371	-0.608643	0.475098	-0.109044
2	14.660767	0.101065	0.204118	-0.202202	0.042771
3	1.750654	0.185155	0.299794	-0.240346	0.046968
4	165.763926	0.191665	-0.277448	0.133514	-0.021280
$P_w/P_c = 1/8$, $P_w + P_c = 1$ atm (corresponding to dry flue gas recycling, FGR)					
1	0.051237	0.515415	-0.618162	0.430921	-0.092082
2	0.688383	0.199807	0.298581	-0.265758	0.052910
3	13.763205	0.138767	-0.001851	-0.049353	0.013012
4	289.841885	0.087511	-0.067295	0.013489	-5.54E-06
$P_w/P_c = 1/4$, $P_w + P_c = 1$ atm					
1	0.052694	0.486247	-0.644137	0.485654	-0.107808
2	0.752776	0.213959	0.306543	-0.264417	0.051889
3	11.543306	0.181991	-0.020460	-0.053791	0.015058
4	252.938841	0.106180	-0.096088	0.028114	-0.002443
$P_w/P_c = 1/2$, $P_w + P_c = 1$ atm					
1	0.052378	0.383225	-0.510937	0.442201	-0.106398
2	0.712283	0.251481	0.161562	-0.150405	0.028982
3	8.067637	0.208239	0.070697	-0.135668	0.032090
4	195.892573	0.147259	-0.156339	0.057698	-0.007266
$P_w/P_c = 3/4$, $P_w + P_c = 1$ atm					
1	0.051639	0.255953	-0.276222	0.311285	-0.084903
2	0.617739	0.340392	-0.126902	0.051357	-0.010259
3	6.051770	0.160253	0.289548	-0.284144	0.060344
4	150.875915	0.201452	-0.233937	0.095159	-0.013302
$P_w/P_c = 1/1$, $P_w + P_c = 1$ atm (corresponding to wet FGR)					
1	0.051487	0.164048	-0.087793	0.195253	-0.063573
2	0.571797	0.412652	-0.339810	0.197886	-0.038963
3	5.398936	0.112364	0.450929	-0.388486	0.079862
4	130.622859	0.238339	-0.288619	0.121962	-0.017651
$P_w/P_c = 2/1$, $P_w + P_c = 1$ atm (corresponding to, e.g., oxy-fuel combustion of natural gas, without FGR)					
1	0.054480	-0.002188	0.286129	-0.048594	-0.016243
2	0.555304	0.546857	-0.714799	0.452812	-0.088841
3	5.040174	-0.001911	0.764177	-0.581819	0.115069
4	100.372663	0.317219	-0.415470	0.186570	-0.028335
$P_w/P_c = 4/1$, $P_w + P_c = 1$ atm					
1	0.060800	-0.053999	0.434975	-0.152413	0.005094
2	5.608831	-0.094953	0.952010	-0.696161	0.136316
3	0.676040	0.606525	-0.853216	0.545562	-0.107328
4	84.540632	0.369661	-0.517493	0.244011	-0.038451

P_w, P_c and P_w/P_c are never constant throughout any real combustion system. The parameters of different representative conditions will be used based on local gas conditions in the combustion system under modeling.



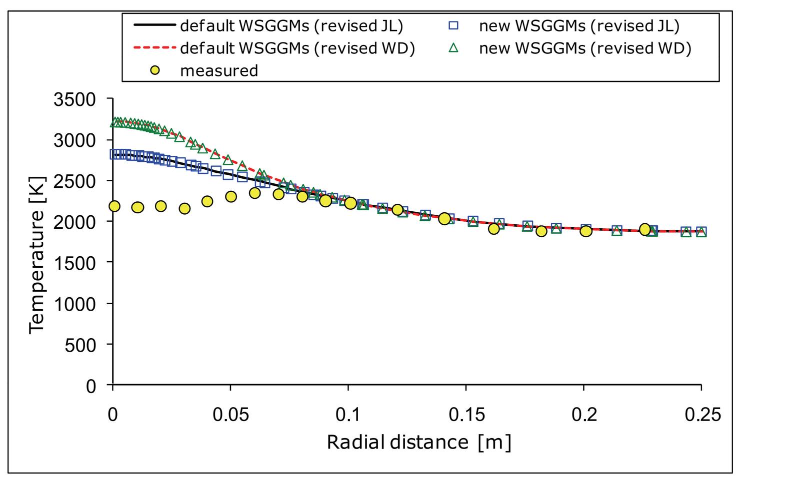
Emissivity vs. beam length at different P_w/P_c, for constant temperature 1750K.

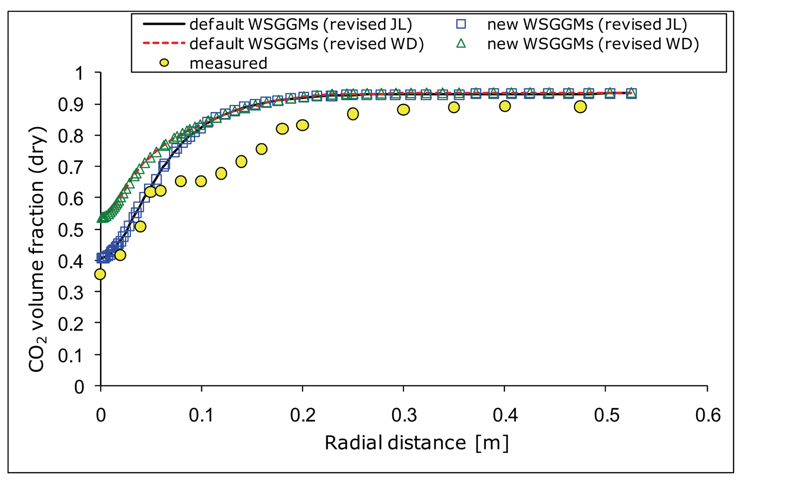


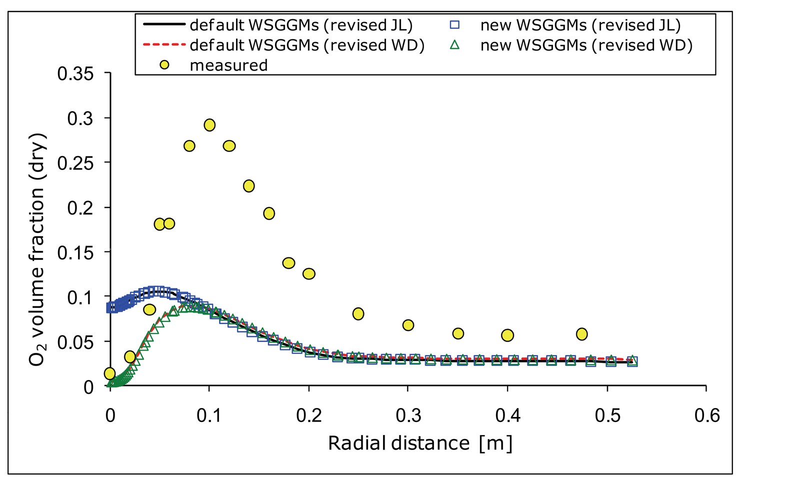
Emissivity vs. gas temperature at different P_w/P_c, for constant beam length 40m.

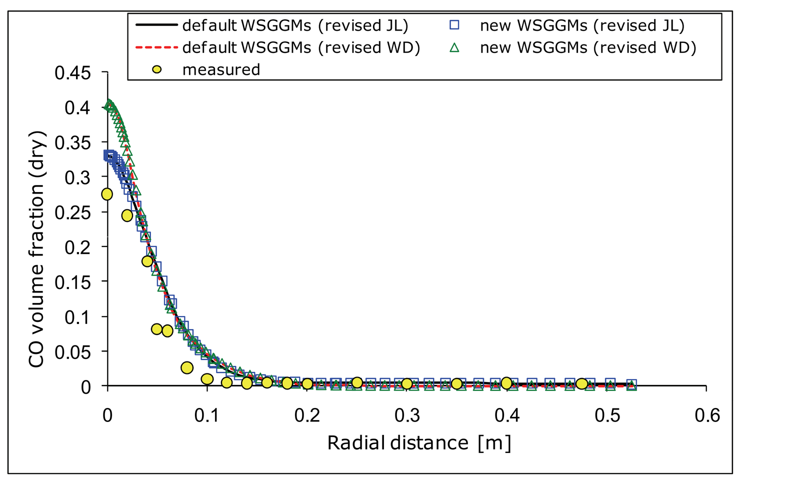
Result 3: Demonstration

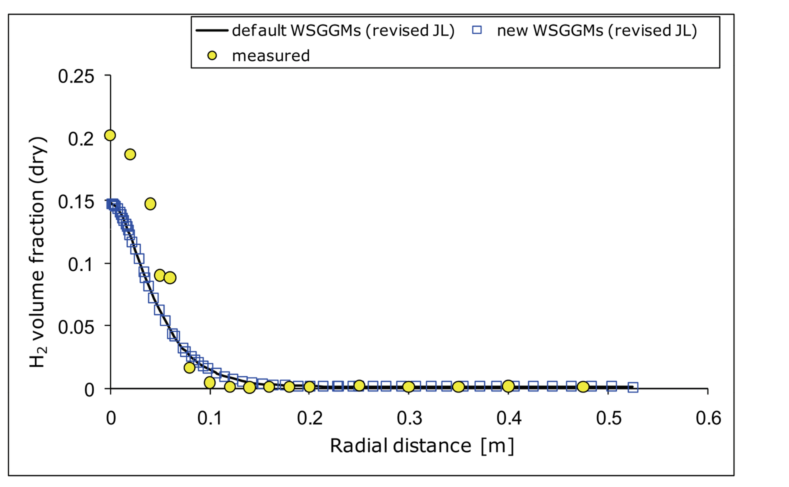
The new models have been applied to CFD of a 0.8MW IFRF oxy-natural gas flame furnace.











Conclusions

The new WSGGMs need to be used in CFD modeling of large-scale oxy-fuel furnaces. For small-scale facilities, they do not make remarkable difference. Combustion chemistry also plays a key role in oxy-firing modelling.

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